U.S. DEPARTMENT OF ENERGY

Nanoscale Controls on Geologic CO_2

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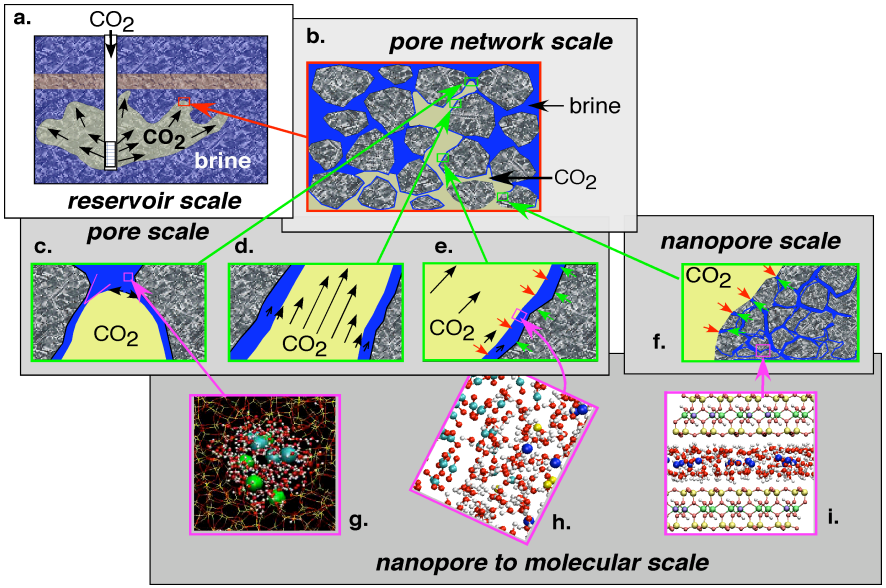
OBJECTIVES are to (1) develop molecular, nano-scale, and pore network scale approaches for controlling flow, dissolution, and precipitation in subsurface rock formations during emplacement of supercritical CO_2; and (2) achieve a new level of prediction of long-term performance



RESEARCH PLAN AND DIRECTIONS: Properties and interactions of complex fluids and minerals must be determined at elevated temperature and pressure, and effects at interfaces and in confined nano-scale pore spaces understood. Novel experimental and computational approaches, and unique DOE experimental facilities (including ALS, SNS, NERSC, Molecular Foundry) will be used.

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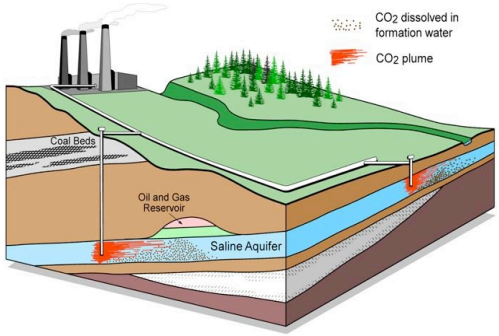
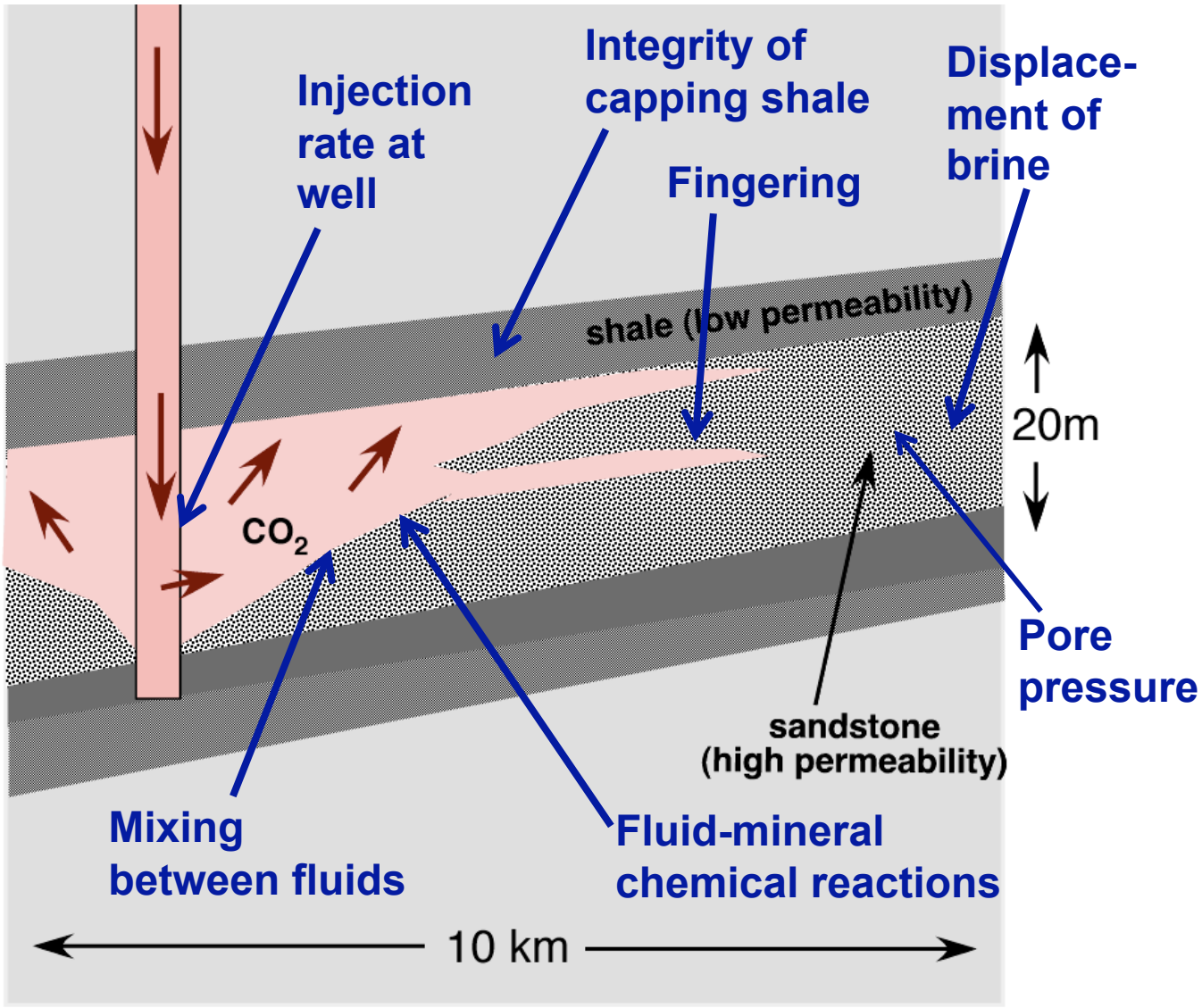
Issues in Geologic Carbon Sequestration

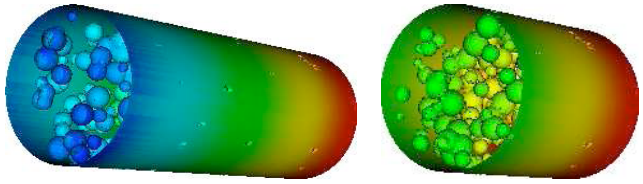


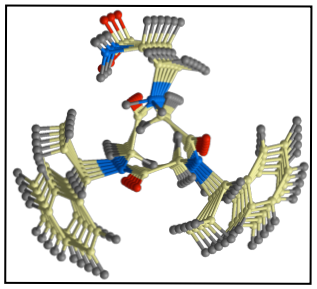
The are a number of things that could cause problems; what will the options be?

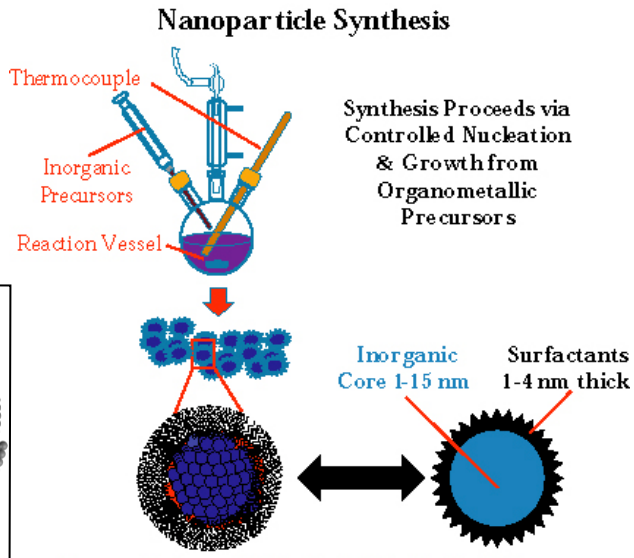


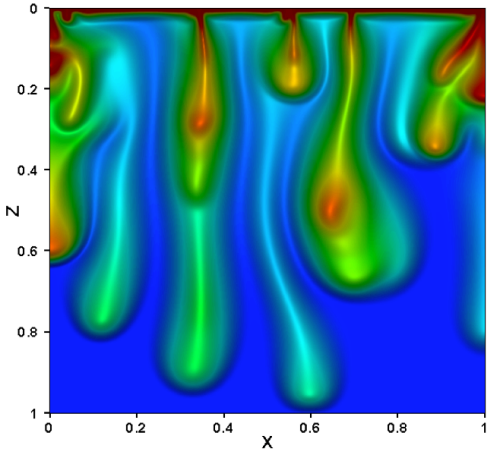
Proposed Research Thrust Areas

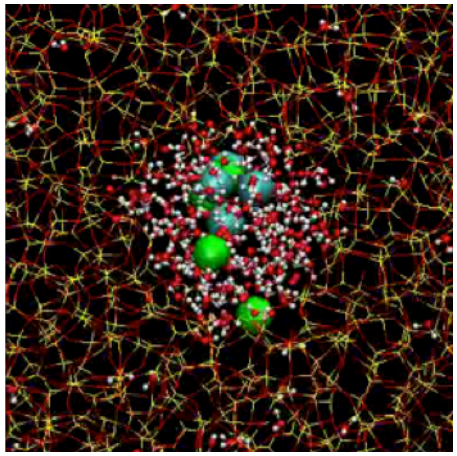
- ***Thrust Area 1: Controlling carbonate mineral nucleation and growth***
- ***Thrust Area 2: Structure, dynamics, and transport of fluids in nanopores and thin films***
- ***Thrust Area 3: Emergent processes***

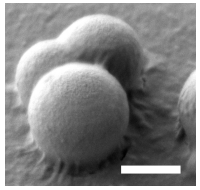


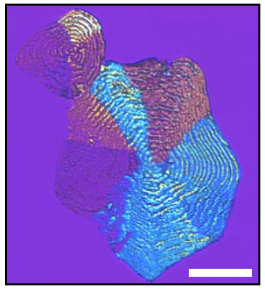


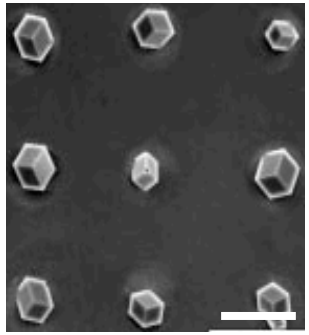




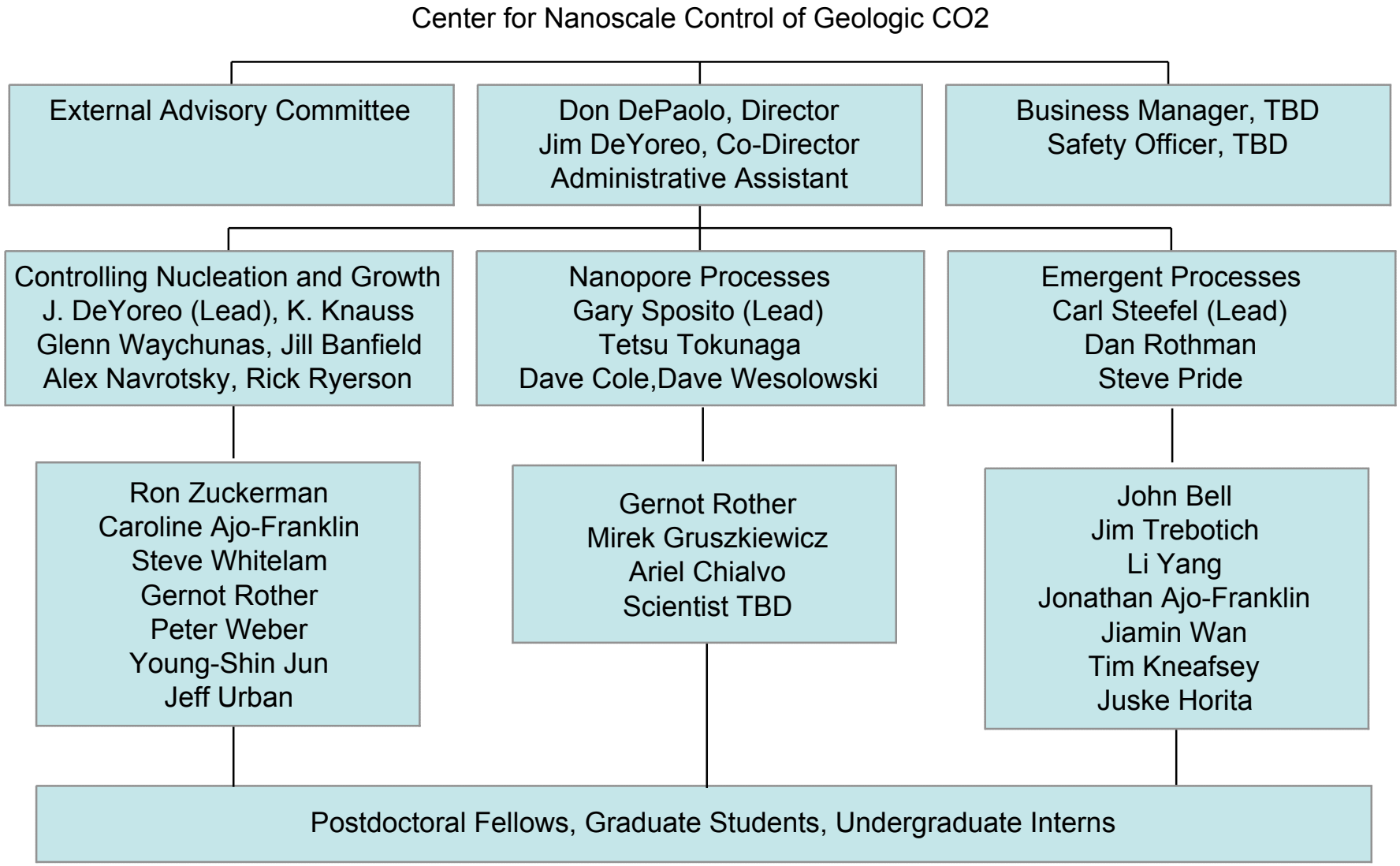




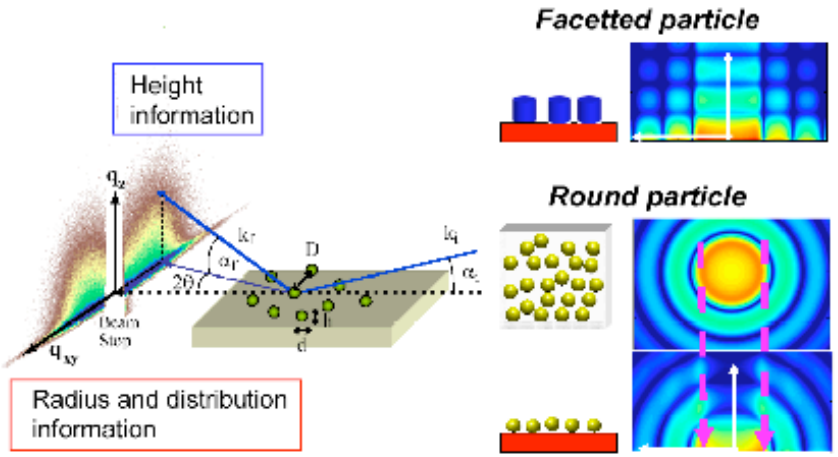


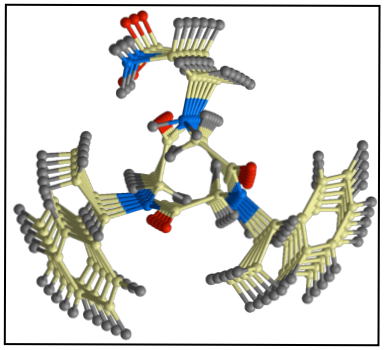


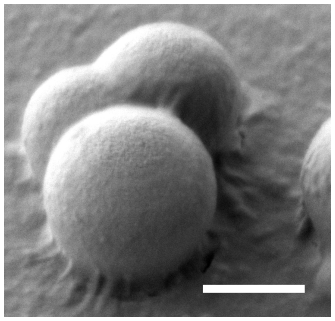
Organization of the EFRC

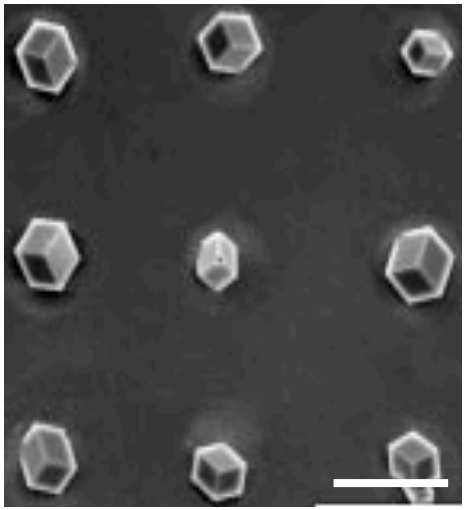


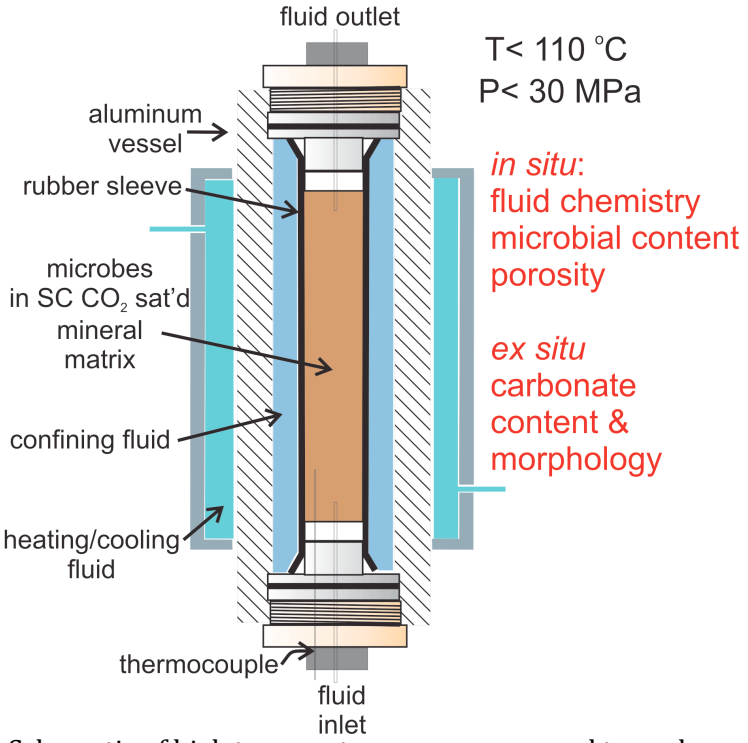
Controlling carbonate mineral nucleation and growth





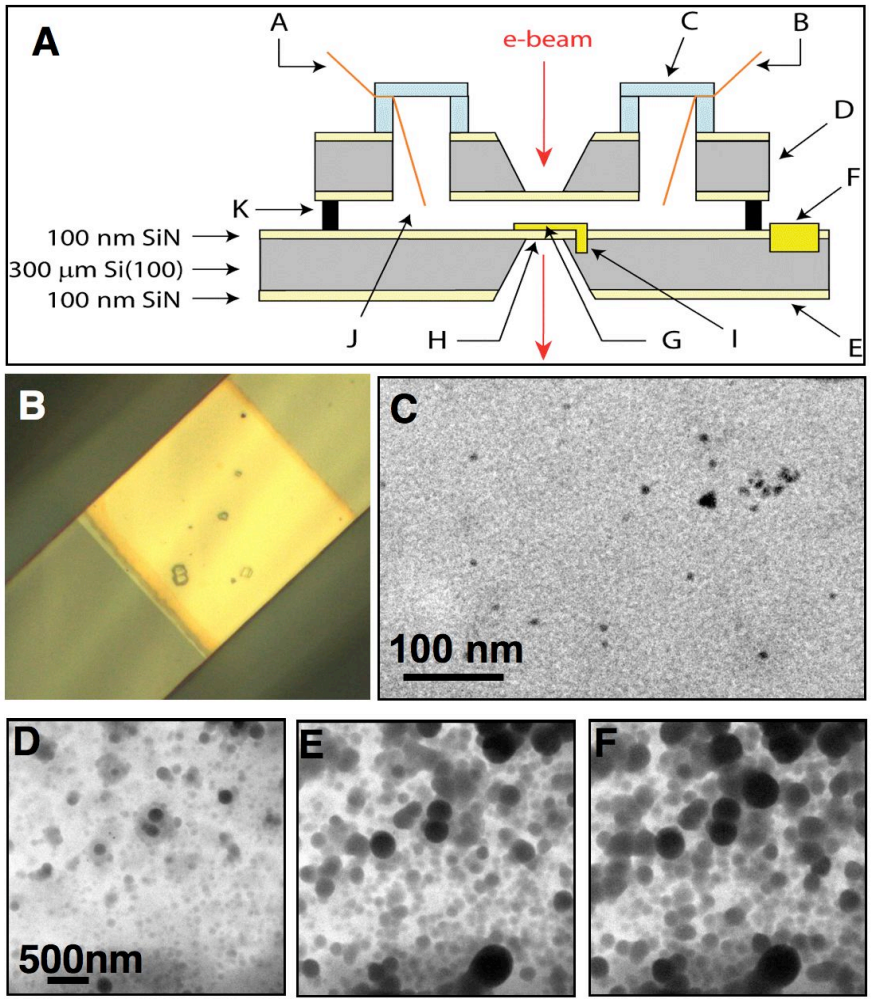


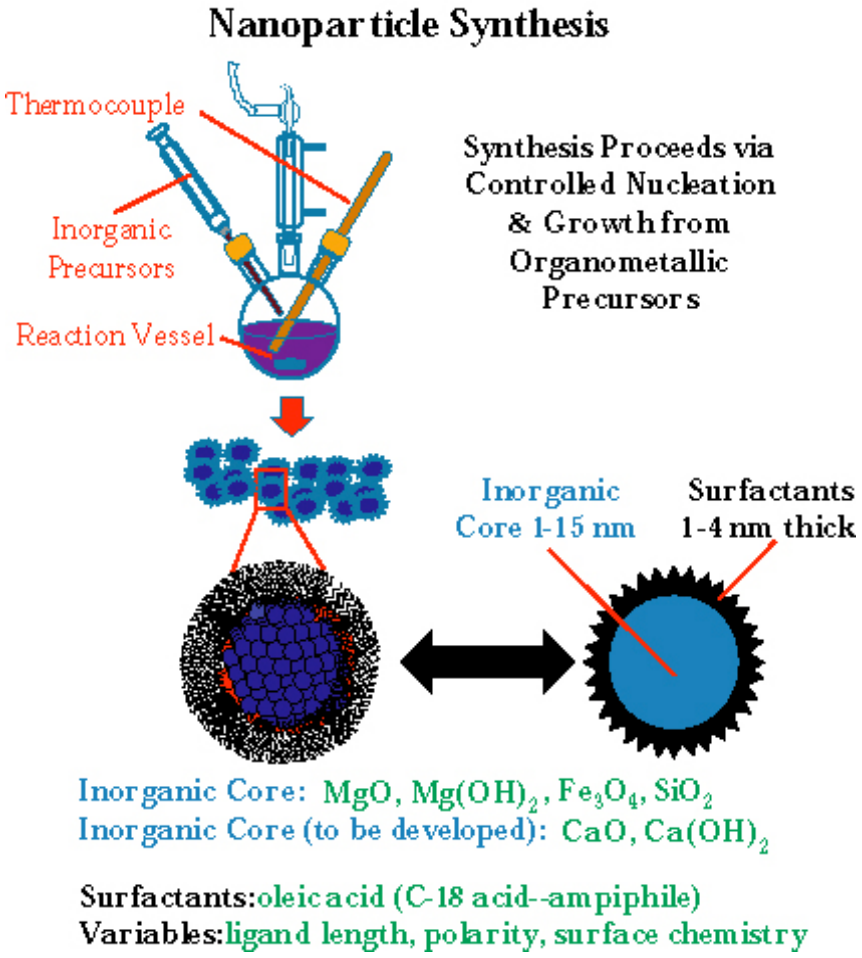




Schematic of high temperature, pressure vessel to probe microbial growth and geochemical effects under sequestration-like conditions.

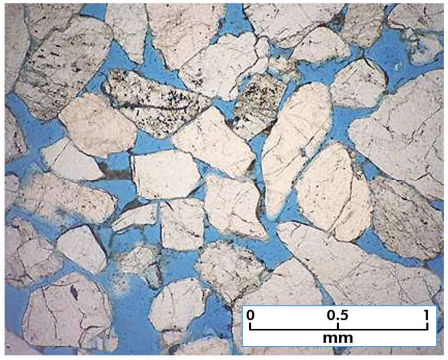
Controlling carbonate mineral nucleation and growth

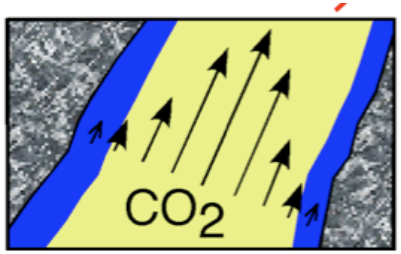


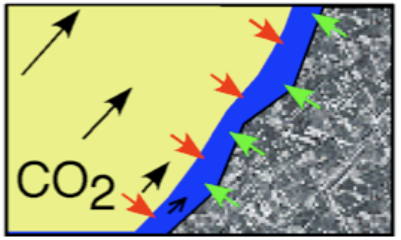


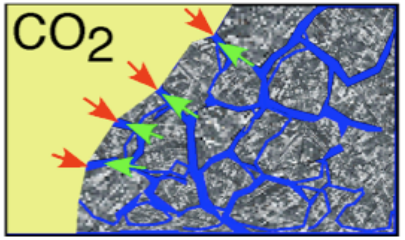
$Ca^{2+}(aq) + HCO_3^{2-}(aq) = CaCO_3(s) = H^+(aq)$

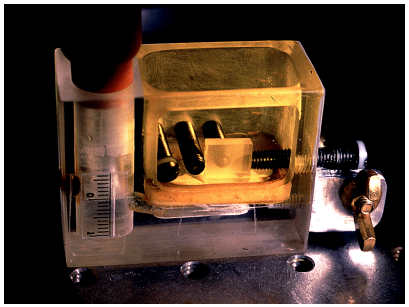
Structure, dynamics, and transport of fluids in nanopores and thin films

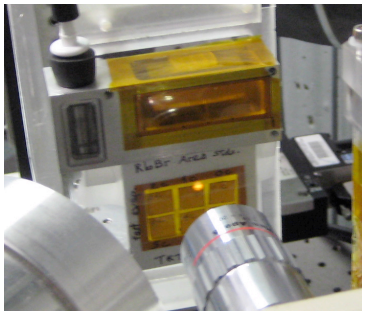


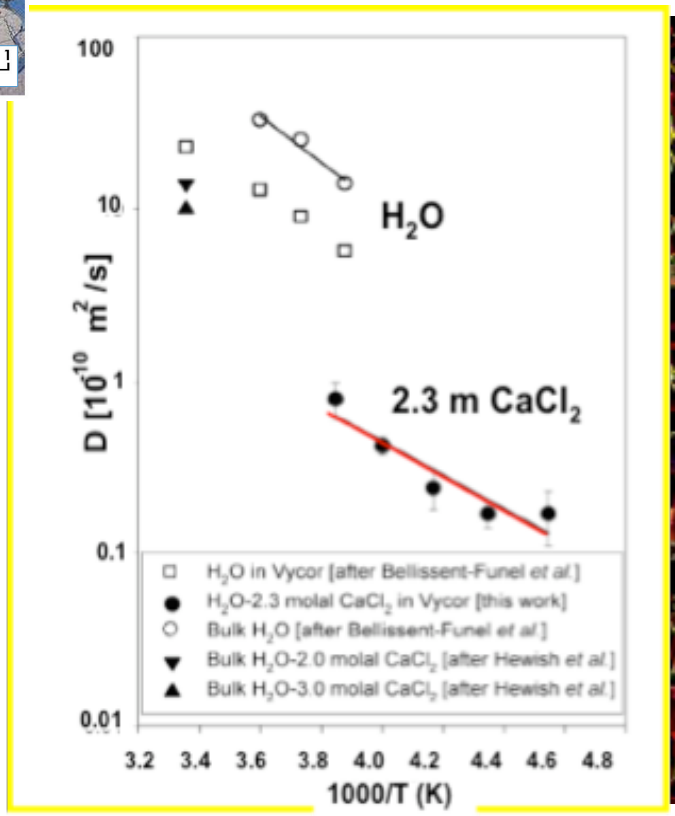


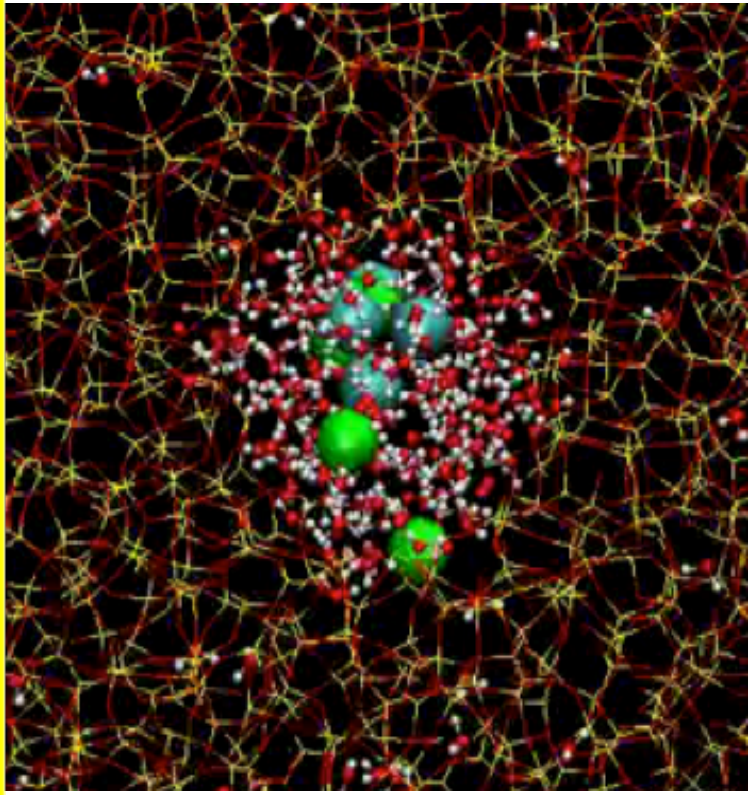




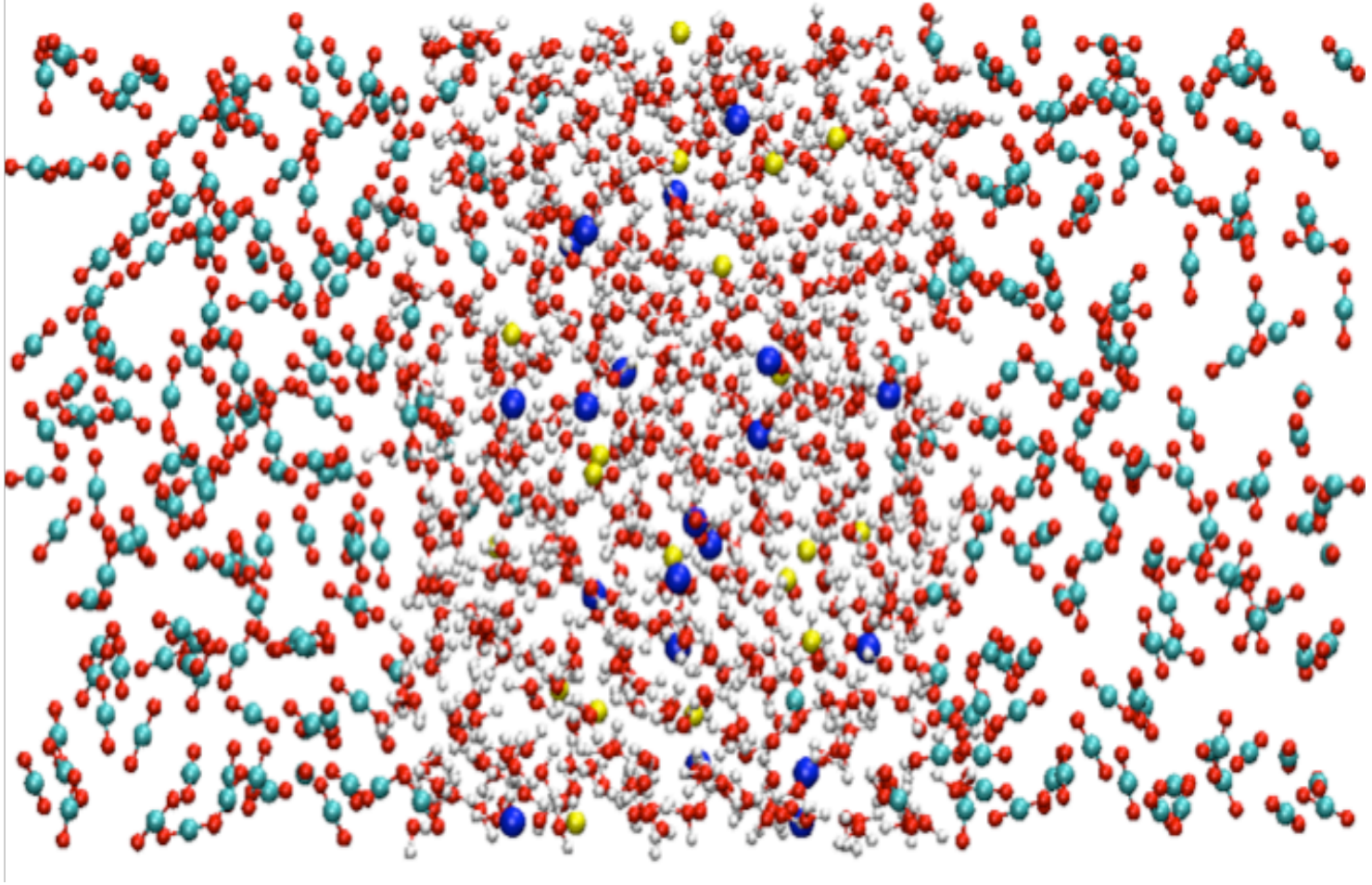






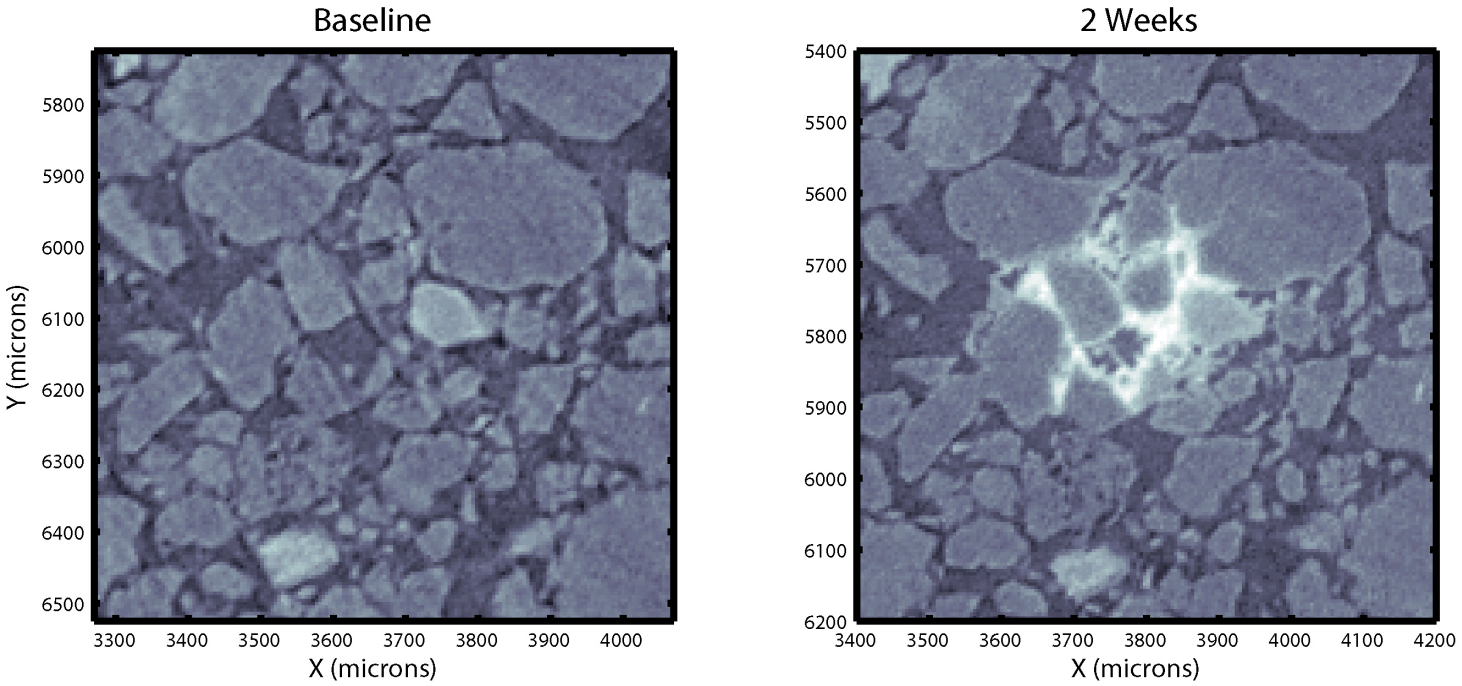


Structure, dynamics, and transport of fluids in nanopores and thin films



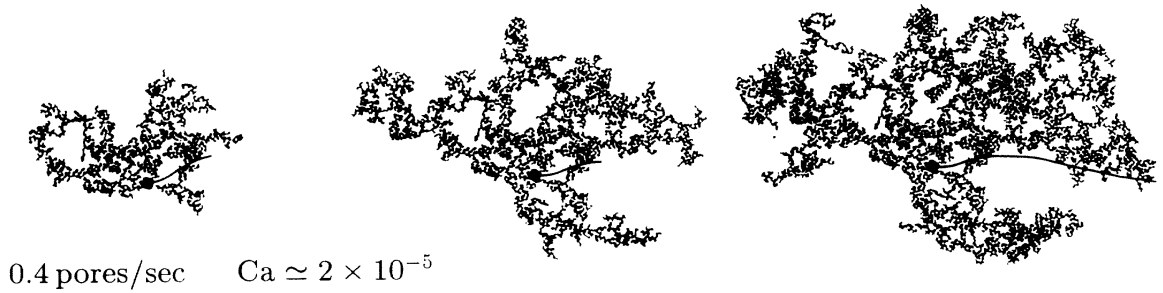
Snapshot of MD simulation of supercritical CO_2 in contact with 2 M NaCl brine. Periodically-replicated simulation cell contains 572 water molecules, 20 Na^+ and Cl^- ions, and 288 CO_2 molecules (red: oxygen, white: hydrogen, green: carbon, blue: sodium, yellow: chloride). Note that CO_2-water interface is not sharp and that few CO_2 molecules are dissolved.

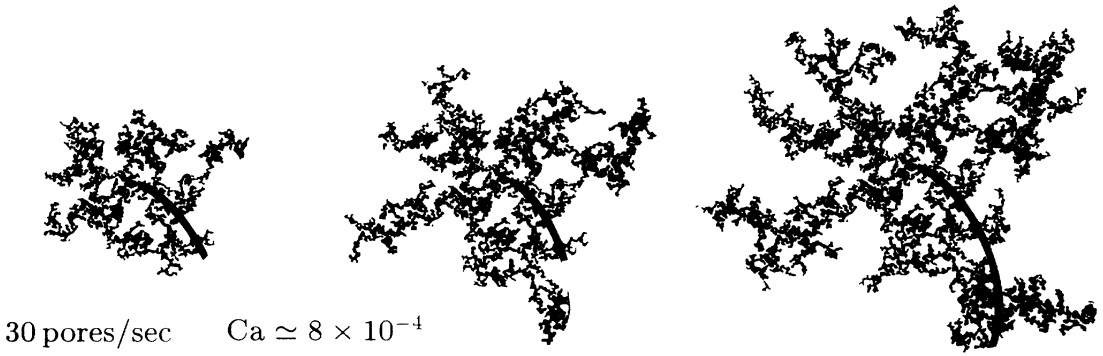
Emergent Processes - Precipitation

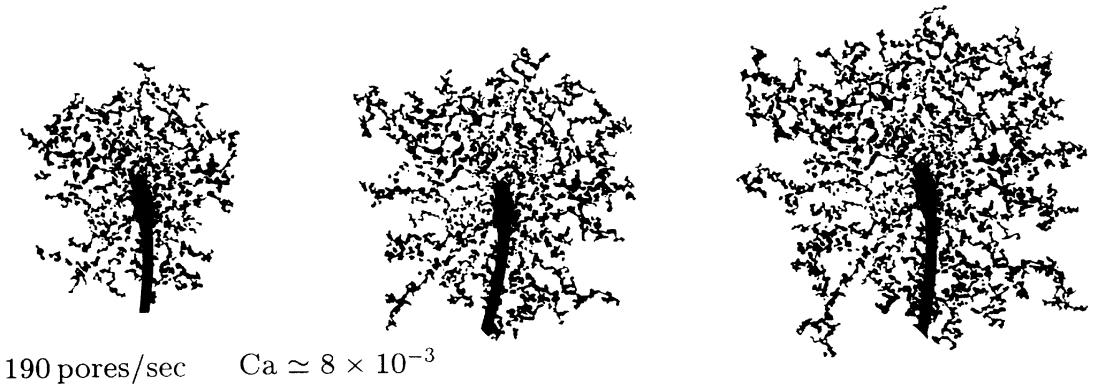


Calcite precipitation (white) within a porous sand imaged using XCT at beamline 8.3.2 ALS, LBNL.

Emergent Processes - Invasion

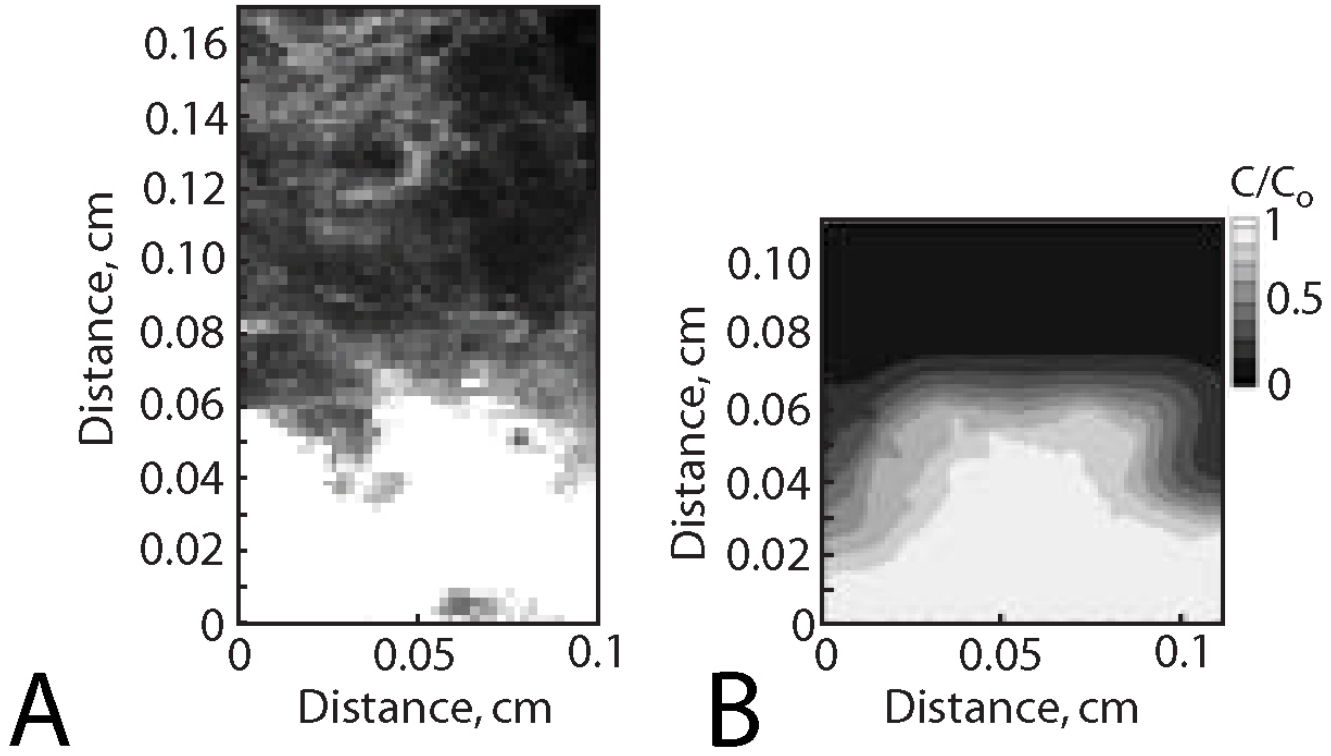






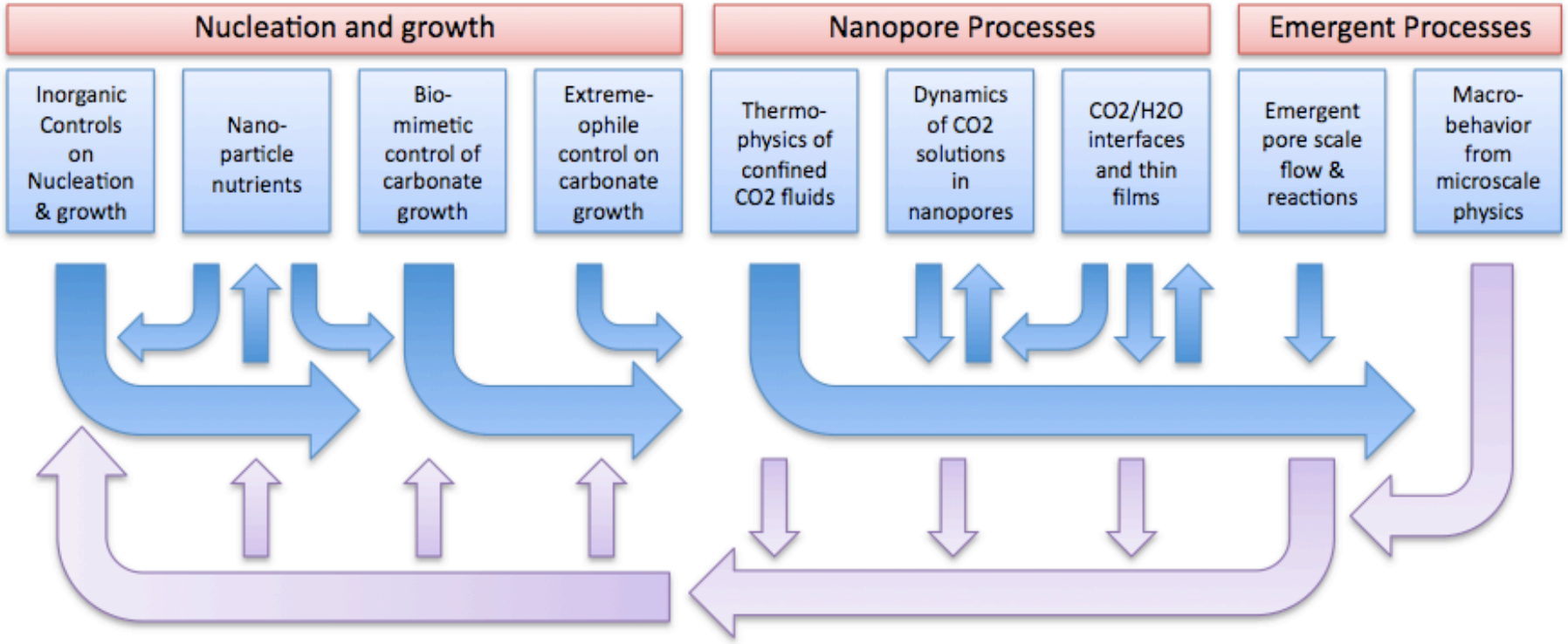
Photographs of an invading fluid (black) being injected from the tip of a tube into a packing of 100 micronμm Plexiglas beads in a Hele-Shaw cell. The invader is nonwetting. The defender has an index of refraction matched to the beads and is thus transparent. From Frette et al. (1994).

Emergent Processes - Diffusion



Tracer diffusion through weathered basalt. Effective continuum-scale diffusivity as a function of extent of weathering was determined from both: A. XRF image of bromide (light) imaged with Beamline 10.3.2 at the ALS, LBNL; B. 3D numerical simulation of front position using a pore network constructed from XCT data using Beamline 8.3.2 at the ALS. From Sitchler et al., 2008.

Research Integration



The proposed research lends itself to integration, in that the studies of nanoscale phenomena both depend on the results of studies of molecular-scale processes, and will help define the most important objectives of those studies. Similarly, the pore-network-scale research depends on the nanoscale results and helps define the most important issues at the nanoscale.